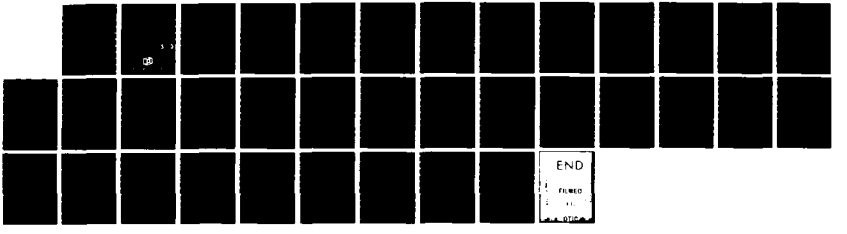
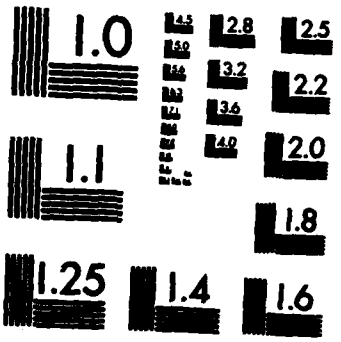
AD-A130 223 CONTINUED INVESTIGATION OF THE ATOMIC PHYSICS OF FLASHLAMP PUMPED CESIUM-NEON LASERS(U) BEERS ASSOCIATES INC RESTON VA C CHANG MAY 83 BEERS-1-83-70-15 1/1

UNCLASSIFIED N00014-82-C-2195 F/G 20/5 NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

(12)

CONTINUED INVESTIGATION OF THE ATOMIC PHYSICS OF FLASHLAMP PUMPED CESIUM-NEON LASERS

- Final Report -

Prepared by:

Ching-Sung Chang

BEERS ASSOCIATES, INC.
Post Office Box 2549
Reston, Virginia 22090

Prepared for:

NAVAL RESEARCH LABORATORY
Washington, D.C. 20375

BEERS 1-83-70-15

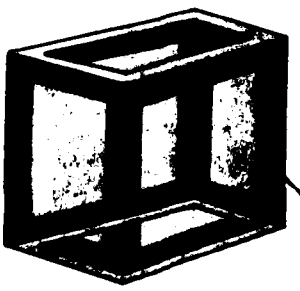
May, 1983

AD A130223

DTIC ELECTE S JUL 8 1983 D A

DTIC FILE COPY

This document has been approved for public release and sale; its distribution is unlimited.



BEERS ASSOCIATES

88 05

TABLE OF CONTENTS

N00014-82-C-2195

Accession For
NTIS GRA&I
DTIC TAB
Unannounced
Justification
By
Distribution/
Availability Codes
Dist | Avail and/or Special
A

DTIC COPY INSPECTED 2

I. Introduction and Summary.

The present report is a continuation of an earlier work involving some issues on a Cs-Ne high power flashlamp and its modeling.[1] Because of the complexity of the physics encountered in an arc discharge of high gas pressures and low voltages, it is necessary to divide the theoretical effort into two parts: microscopic and macroscopic processes. A detailed discussion of this modeling has been given separately in a status report.[2]

In the present report, we are primarily concerned with atomic processes in a high pressure gas discharge. The theoretical endeavour is highlighted in a detailed calculation of spectral line profiles, which are essential to meaningfully model an arc lamp performance. We also examine the effect of neon as a buffer gas in a high pressure cesium discharge tube. Under the condition of comparable cesium and neon pressures, we concluded that neon buffer gas is beneficial to the overall lamp performance. The detailed discussion can be found in Reference 2.

This report is devoted to a rigorous analysis and calculations of spectral line shapes for high pressure and low voltage arc lamp applications. In Section II, a theoretical description of spectral line shape analysis is given. The formultion used is a straightforward generalization of those used in a previous report.[1] Section III describes spectral line shape analysis and calculations. The calculations include the following four types of interaction:

- neutral-neutral interactions: Cs-Cs and Cs-Ne,
- neutral-charged interactions: Cs-e and $Cs-Cs^{+}$.

These collisions lead to broadenings, shifts, and asymmetrics of the observed spectral line shapes and to the occasional appearance of diffuse bands.

In Section IV, our future research plans and recommendations are indicated. Finally, a listing of the code developed for applying the given model is presented in Appendix A followed by a detailed mathematical derivation

of spectral line shapes in Appendix B*.

Based on our limited efforts, we summarize our theoretical findings as follows:

- for high power Cs-Ne flashlamps, the neon pressure should be comparable to cesium pressure,
- if neon (or other inert gases) pressure is several orders of magnitude higher than cesium (or other alkali atoms) pressures, an infrared laser seems possible by optical pumping methods, and
- for high power Cs-Ne arc lamps, the spectral profile is mainly determined by cesium doublet mixing effect.

II. Theoretical Description.

The study of spectral line shapes was actively pursued during the past fifty years. Numerous review articles and books have been written since late 1930.[3,4] Regardless of theoretical approaches taken in the previous work, it is assumed that an interaction potential between a radiating particle (atom or molecule) and a perturbing particle as a function of interparticle distance is known. As a result, experimental measurements of spectral line shapes are used to determine the parameters introduced in the assumed interaction potential. This method, however, achieved only a limited success. Several attempts were made in recent years to fit experimental line shapes by introducing more and more adjustable parameters into the existing thoery.

The effort of this kind is, however, fruitless in our opinion. The reason is simple. First of all, the interaction potential cannot, in general, be represented as a function of particle separations in a simple mathematical form.[5] Secondly, from a rigorous theoretical point of view

---

* Appendix B not reproduced in all copies of this report.

it would be highly unsatisfactory because of its lack of predictability if it should contain adjustable parameters.

In order to circumvent the deficiency as stated above, a new approach must be developed. The method of calculating spectral line shapes to be given below has two important advantages over the previous approach. Firstly, no assumed form of interaction potential as a function of inter-particle separation is used. Secondly, the formulation can be easily extended to interactions involving various different species as lons as the interaction is of electromagnetic origin. As a consequence, the resulting line shape does not contain any adjustable parameters. It is completely determined by the atomic or molecular structures of the radiating and perturbing particles.

Calculations of spectral line shapes can be accomplished by a simple concept. For an atom or a molecule initially in a given excited state making a radiative transition to a lower quantum state, a photon is emitted. The frequency distribution of the emitted photon for a given transition is called a spectral line shape. For a single isolated atom without any external perturbation, the line shape can be derived using the well-known method of Weisskopf and Wigner.[6] This method can be generalized to the problem including the external perturbations due to interaction with other atoms of the same or different species. The effect of external perturbation is to modify the upper and lower radiating states. In the following section, we indicate how to carry out an explicit calculation of spectral line shapes.

III. Spectral Line Shape Analysis and Calculations

We shall consider the far-infrared radiation from the cesium atom in the wavelength range between 1μ and 5μ. These radiations involve 7S → 6P, 7P → 5D and 5D → 6P as transitions. These transitions do not involve the ground state 6S as the lower level. Thus the photon dispersion is likely to be unimportant. Assuming this to be the case, we may approximate

$$\omega_{\vec{k}} = |\vec{k}| \equiv \omega.$$

As a consequence, the photon wavefunction renormalization constant $Z_3(\omega_{\vec{k}})$ is equal to unity, and Equation (6)* becomes, using the nonrelativistic approximation,

$$K^{\alpha\alpha}_{n,n'}(\vec{k}_\lambda) = e\,(2\omega V)^{-1/2} \langle n|\frac{\vec{p}_\alpha}{m} \cdot \hat{e}_\lambda\, e^{i\vec{k}\cdot\vec{x}}|n'\rangle \,. \tag{III.1}$$

The electron-atom interaction kernel $K^{\alpha\beta}$ in the same approximation can be written, neglecting $P_\gamma(q,q_0)$

$$K^{\alpha\beta}_{n_1 n_2}(\vec{p},\vec{q}) = -\frac{4\pi e^2}{V} \langle n_1|e^{i\vec{q}\cdot\vec{x}}-1|n_2\rangle/(\vec{q}^2-q_0^2) \Big|_{q_0=\Delta n_1,n_2 + \frac{i}{2}\gamma_{n_1}} \tag{III.2}$$

The atom-atom interaction kernel $K^{\alpha\alpha}$ can likewise be obtained,

$$K^{\alpha\alpha}_{n_1,n_2,n_3,n_4}(\vec{P},\vec{Q}) = -\frac{e^2}{V} \langle n_1|\gamma_\mu e^{i\vec{Q}\cdot\vec{X}}|n_2\rangle \langle n_3|\gamma_\mu e^{-i\vec{Q}\cdot\vec{X}}|n_4\rangle$$

$$\times \left[(\delta^{n_1,n_2}_{\vec{P},\vec{Q}})^2 - \vec{Q}^2\right]^{-1} \,. \tag{III.3}$$

If now we use the dipole approximations, Equations (III.1-III.3) take the form

---

* Equations (1)-(90) refer to Equations in Appendix B.

$$K^{\alpha\gamma}_{n,n'}(\vec{k}_\lambda) = \frac{\Delta_{n,n'}}{\sqrt{2\omega V}} \vec{d}_{n,n'} \cdot \hat{e}_\lambda$$

$$K^{\alpha\beta}_{n,n'}(\vec{p},\vec{q}) = \frac{e}{V} \vec{q} \cdot \vec{d}_{n,n'}/q^2$$

$$K^{\alpha\alpha}_{n_1,n_2,n_3,n_4}(\vec{P},\vec{Q}) = \frac{1}{V} [\Delta_{n_1,n_2}\Delta_{n_3,n_4}(\vec{d}_{n_1,n_2} \cdot \vec{d}_{n_3,n_4}) - (\vec{d}_{n_1,n_2} \cdot \vec{Q})$$

$$\times (\vec{d}_{n_3,n_4} \cdot \vec{Q})][(\delta^{n_3,n_4}_{\vec{P},\vec{Q}})^2 - \vec{Q}^2]^{-1} ,$$

where d_{n_1,n_2} is the dipole moment defined as

$$d_{n_1,n_2} = \frac{e}{\sqrt{4\pi}} \langle n_1|r|n_2\rangle .$$

We shall use the above approximation to analyze the quantities appearing in our lineshape formula. The quantity γ_e in Equation (64) is due to the photon-atom interaction, which is obtained from Equation (33). Explicitly,

$$\gamma_e = \frac{4}{3} \sum_n |\Delta_{e,n}|^3 |\vec{d}_{e,n}|^2 \theta (E^\alpha_e - E^\alpha_n)$$

which is a sum of Einstein A-coefficients for dipole allowed transitions to the lower states.

The quantities that appear in Equations (69) and (73) are due to electron-atom and atom-atom interactions. From Equations (73), letting $\Omega = 0$, we have

$$\left.\begin{aligned} \tilde{\Gamma}^j_{\alpha\alpha}(o) \equiv A^j_{\alpha\alpha}(P_o) &= \rho_\alpha \sum_{n',n''} \int d^3P f(P) W^{j,n',n''}_{\alpha\alpha}(\vec{P},\vec{P}_o) \\ \tilde{\Gamma}^j_{\alpha\beta}(o) \equiv A^j_{\alpha\beta}(P_o) &= \rho_\beta \sum_{n'} \int d^3p g(p) W^{j,n'}_{\alpha\beta}(\vec{p},\vec{P}_o) \end{aligned}\right\} \qquad \text{(III.4)}$$

where

$$W^{j,n',n''}_{\alpha\alpha}(\vec{P},\vec{P}_o) = \int \frac{d^3Q}{(2\pi)^3} \frac{|K^{\alpha\alpha}_{g,j,n',n''}(Q)|^2}{\Delta_{n',j}+\Delta_{n'',g}-\delta^o_{\vec{P},\vec{Q}}-\frac{i}{2}\gamma_j}$$

$$W^{j,n'}_{\alpha\beta}(\vec{p},\vec{p}_o) = \int \frac{d^3q}{(2\pi)^3} \frac{|K^{\alpha}_{j,n}(q)|^2}{\varepsilon_{\vec{p}+\vec{q}}-\varepsilon_{\vec{p}}+\Delta^{n',j}_{\vec{q}}-\frac{i}{2}\gamma_j} \qquad \text{(III.5)}$$

In Equation (III.4), g(p) is the electron distribution function, which is assumed to be Maxwellian with an electron temperature T_β ,

$$g(\vec{p}) = (\pi p_\beta^2)^{-3/2} e^{-\vec{p}^2/p_\beta^2}$$

$$p_\beta = (2 m k_B T_\beta)^{1/2}$$

The effect of electron drift velocity will be ignored. Both functions defined in Equation (III.5) are complex with positive imaginary parts, with γ_j being the radiative decay width of the radiating state $|j>$. The interaction kernels $|K^{\alpha\alpha}|^2$ and $|K^{\alpha\beta}|^2$ are functions of Q and q respectively. They are independent of $\vec{P}$ and $\vec{P}_o$. Furthermore, f(p) and g(p) are also independent on the direction of $\vec{P}$ and $\vec{p}$. As a consequence, the angular integrations in Equations (III.4) and (III.5) can be carried out. Let

$$A(P_o) = 2\mu \int d^3P\, f(P) \int \frac{d^3Q}{(2\pi)^3} \frac{|K(Q)|^2}{Q^2+2(\vec{P}-\vec{P}_o)\cdot\vec{Q}+a}$$

where

$$\text{Im } a < 0 .$$

Carrying out the angular integrations, we get

$$A(P_o) = \frac{\mu}{2\pi P_o}\int_{-\infty}^{\infty} PdPf(P)\int_{-\infty}^{\infty} QdQ|K(Q)|^2 \quad [|P+P_o|+\frac{1}{2}(Q+\frac{a}{Q})]\ln(Q^2+2Q|P+P_o|+a) \tag{III.6}$$

If f(P) is assumed to be Maxwellian as in Equation (79), then Equation (III.6) the form

$$A(P_o) = \frac{\mu}{(2\pi)^{5/2}P_o P_\alpha}\int_{-\infty}^{\infty} dPe^{-P^2/p_\alpha^2}\frac{P+P_o}{|P+P_o|}B(|P+P_o|) \tag{III.7}$$

where

$$B(x) = \int_{-\infty}^{\infty} QdQ|K(Q)|^2 \ln(Q^2+2Qx+a) \tag{III.8}$$

Consider the electron-atom interaction. If the dipole approximation is made, then

$$|K(Q)|^2 \propto Q^{-2}$$

The integrand in Equation (III.8) behaves as for large Q,

$$\ln Q/Q$$

and the integral diverges. The divergence of this kind is encountered in the usual thoery based on a multipole expansion of the static coulomb potential, and adjustable parameters are often invoked to make the results finite.

In the present formulation, this divergence is seen from the approximation of the matrix elements of the form

$$\langle n_1 | e^{iQz} | n_2 \rangle \cong i\, Q \langle n_1 | z | n_2 \rangle$$

This approximation is correct only when Q is small. For large Q, the matrix element must decrease at least as Q^{-1} according to the Riemann-Lebesgue lemma. Because of this fact, we showed in an earlier report that we may approximate

$$\langle n_1 | e^{iQz} | n_2 \rangle \cong i\, Q \langle n_1 | z | n_2 \rangle / [1 + \frac{Q^2}{6} | \langle n_i | z | n_2 \rangle |^2] \qquad \text{(III.9)}$$

If Equation (III.9) is used to evaluate electron excitation cross sections, an agreement with experimental data is achieved. Note that Equation (III.9) is consistent with the expected Q-dependence for both large and small Q.

If now we used Equation (III.9) to evaluate $|K(Q))|^2$, than

$$|K(Q)|^2 \propto \frac{1}{Q^2(1 + bQ^2)^2} \qquad \text{(III.10)}$$

The integral in Equation (III.8) thus converges rapidly for large Q. Note that there is a logarithmic singularity in Equation (III.8) at Q = 0 if Equation (III.10) is used. This arises from the Q^{-2} dependence in the electron-atom interaction kernel where the lifetime of the coupled radiating state $|j\rangle$ has been ignored. If this finite lifetime and retardation effect are taken into account, then Q^{-2} should be replaced by

$$[Q^2 - (\Delta_{j,n'} - \tfrac{i}{2} \gamma_j)^2]^{-1}$$

and the logarithmic singularity on the real axis disappears.

For atom-atom interaction, we have, if dipole approximations are used,

$$|K(Q)|^2 = 0 \quad (1)$$

for large Q. Then the integral in Equation (III.8) diverges quadratically. However, using Equation (III.9) and taking into account the finite life-time of the radiating state, a well-defined finite physical result is again obtained.

According to the foregoing discussion, the functions $|K(Q)|^2$ in Equation (III.8) have the following forms:

- Electron-atom interaction

$$|K(q)|^2 = e^4|\langle j|z|n'\rangle|^2 q^2 \{[(q-\Delta_{j,n'})^2 + \frac{\gamma_j^2}{4}][(q+\Delta_{j,n'})^2 + \frac{\gamma_j^2}{4}]$$

$$\times (1 + \frac{1}{6}|\langle j|z|n'\rangle|^2 q^2\}^{-1} \qquad \text{(III.11)}$$

- Atom-atom interaction

$$\left.\begin{aligned} |K(Q)|^2 &= e^4|\langle j|z|n'\rangle\langle g|z|n''\rangle|^2\, G(Q) \\ G(Q) &= (Q^4 - \Delta_{g,n''}\Delta_{j,n'}Q^2 + 2|\Delta_{g,n''}\Delta_{j,n'}|^2) \\ &\quad \times \{(1 + C_{j,n'}^2 Q^2)^2 (1 + D_{n''}^2 Q^2)^2 [(Q - \Delta_{j,n'})^2 + \frac{\gamma_j^2}{4}] \\ &\quad \times [(Q + \Delta_{j,n'})^2 + \frac{\gamma_j^2}{4}]\}^{-1} \end{aligned}\right\} \qquad \text{(III.12)}$$

$\sqrt{6}\ |\langle j|z|n'\rangle|$)

$\overline{6}\ |\langle g|z|n''\rangle|$)

I.12), averages over dipole orientations have been performed.

present treatment, we also include the retardation effect as in
11) and (III.12). This effect has not been included in existing theories
eshape as far as we know. However, as pointed out by Stevens,[5] the
ect is important in determining the interaction energies between two
separation. This effect should lead to a certain modification on
arameters in particular, and the lineshape itself in general.

e calculation of spectral line profiles can be performed if the
ation (67), are satisfied. In this connection, the lineshape
on (68), may be used. From Equations (74) and (68), may be used.
(74) and (68), after carrying out the angular integration, we

$$)> = \frac{M}{\omega} \ (2\pi p_\alpha^2)^{-3/2} \int_0^\infty dP_o \ P_o \ e^{-P_o^2/p_\alpha^2}$$

$$\times \left[\tan^{-1}\left(\frac{Z + R_1(P_o) + \frac{P_o\omega}{M}}{R_2(P_o)}\right) - \tan^{-1}\left(\frac{Z + R_1(P_o) - \frac{P_o\omega}{M}}{R_2(P_o)}\right)\right] \qquad \text{(III.13)}$$

'e

$$Z = \omega - \Delta_{e,n}$$

:grating Equation (III.13) by parts, we have

$$\langle L_{e,n}(Z)\rangle = \frac{1}{\sqrt{2\pi}\, p_\alpha}\left[\int_{-\infty}^{\infty} dP_o\, e^{-P_o^2/p_\alpha^2}\, \frac{R_2(P_o)}{D_+(P_o,Z)} + J_{e,n}(Z)\right] \tag{III.14}$$

re-

$$\left.\begin{aligned} J_{e,n}(Z) &= \int_0^{\infty} dP_o e^{-P_o^2/p_\alpha^2}\left[\frac{N_+(P_o,Z)}{D_+(P_o,Z)} - \frac{N_-(P_o,Z)}{D_-(P_o,Z)}\right] \\ D_\pm(P_o,Z) &= \left[Z + R_1(P_o) \pm \frac{P_o\omega}{M}\right]^2 + [R_2(P_o)]^2 \\ N_\pm(P_o,Z) &= R_2(P_o)\frac{\partial}{\partial P_o} R_1(P_o) - \left[Z + R_2(P_o) \pm \frac{P_o\omega}{M}\right]\frac{\partial}{\partial P_o} R_2(P_o) \end{aligned}\right\} \tag{III.15}$$

P_o dependence in $R_1(P_o)$ and $R_2(P_o)$ is ignored, Equation (III.14) reduces to the l-known Voigt profile.

To evaluate the integrals in Equation (III.14) as a function of Z, it is :ssary to calculate $R_1(P_o)$ and $R_2(P_o)$, which are expressed in terms of A_e A_n as defined in Equation (69). They are given explicitly below.

Define the reduced masses μ_α and μ_β for atom and electron respectively,

$$\left.\begin{aligned} \frac{1}{\mu_\alpha} &= \frac{1}{M} + \frac{1}{M} = \frac{2}{M} \\ \frac{1}{\mu_\beta} &= \frac{1}{m} + \frac{1}{M} \cong \frac{1}{m} \end{aligned}\right\}$$

We write

$$A_j(P_o) = A_\alpha^j(P_o) + A_\beta^j(P_o)$$

where

$$A_\alpha^j(P_o) = \rho_\alpha \frac{\mu_\alpha}{(2\pi)^{5/2} p_\alpha \tilde{P}_o} \int_{-\infty}^{\infty} dP\, e^{-P^2/p_\alpha^2} \frac{P + \tilde{P}_o}{|P + \tilde{P}_o|} B_\alpha^j(|P + \tilde{P}_o|)$$

$$A_\beta^j(P_o) = \rho_\beta \frac{\mu_\beta}{(2\pi)^{5/2} p_\beta \tilde{P}_o} \int_{-\infty}^{\infty} dp\, e^{-p^2/p_\beta^2} \frac{p + \tilde{P}_o}{|p + \tilde{P}_o|} B_\beta^j(|p + \tilde{P}_o|)$$

The functions $B_\alpha^j(|P + \tilde{P}_o|)$ and $B_\beta^j(|p + \tilde{P}_o|)$ are computed according to Equation (III.8) with the parameters occuring there identified as follows: For B_β^j, use Equation (III.11) for $|K(Q)|^2$, and

$$a \equiv 2\mu_\beta(\Delta_{n',j} - \tfrac{i}{2}\gamma_j), \quad \tilde{P}_o = \frac{m}{M} P_o$$

For B_α^j, use Equation (III.12) for $|K(Q)|^2$, and

$$a = 2\,\mu_\alpha(\Delta_{n',j} + \Delta_{n'',g} - \tfrac{i}{2}\gamma_j), \quad \tilde{P}_o = P_o.$$

The computer program is given in Appendix A. Certain sample calculations are shown in Reference 2.

IV. Future Plans

For a single isolated line, a general expression of spectral line shapes was obtained, as shown in Equation (72) of Appendix B*. Because of the limited funds available at present, a general numerical evaluation of Equation (72) cannot be performed. Only the approximated expression, Equation (68), to the exact formula, Equation (72), was numerically implemented. There are circumstances in which the approximations, Equations (67), leading to Equation (68) may fail.. In this connection, numerical calculations of the exact expression, Equation (72), must be carried out.

In addition to the above technical program aimed at performing an accurate spectral line shape calculation, there are three issues needed to be addressed for future program needs. They are

A. Physics Issues

- Atomic Model Development
- Atomic Core Polarization Effects
- Spectral Line Profile Formation
- Electrical Conductivity Calculation
- Thermal Conductivity Calculation

B. Devise Improvement Issues

- Emission Spectrum Tailoring
- Flashlamp Reliability Improvement
- Optical Gas Mixture
- Cesium-Neon Discharge Laser
- Cesium Vapor Heating Problems

---

* Not reproduced in all copies of this report.

C. Diagnostic Issues

- Discharge Plasma Diagnosis
- EO Systems Quality Control

Detailed discussions of the above issues can be found in Reference 2.

Appendix A

Computer Program Description and Listing

A.1 Program Description

This is a description of the computer routines mentioned in in Section III above which are used to compute line shape by solving equation III.13. The description of the calculations in each routine follows the order of the calculations in that routine. The routines appear in the order that they are called in the program. A flowchart for subroutine SHPE and its associated routines follows in Figure 1.

Subroutine SHPE is the primary routine - it calculates the final lineshape:

Subroutines INTLZ,SETDAT and MED are called to set the physical constants and atomic data.

For each allowed transition between fine structure lines a lineshape is calculated:

Subroutine SETTRN is called to set indices corresponding to to the fine structure lineshape being calculated.

Subroutine RS is called to provide the values of the parameters R1(Po),R2(Po), (from equation III.13), at the Hermite abscissa points.

At each frequency point used to define the lineshape:

The integral in equation III.13 is performed by Hermite integration to produce a lineshape value.

The weighted value is added to the final lineshape at that frequency point.

Subroutine RS calculates the values of the parameters R1(Po),R2(Po) at the Hermite abscissa points:

First the contribution to R1(Po), R2(Po) from the initial atomic state:

Subroutine SET is called to set parameter values corresponding to which atomic state and exciting states are involved.

Subroutine AS is called for each of the species (atoms, electrons, buffer atoms, ions) to provide the values of the parameters Ae,An as defined in equation (69).

Sum the Ae,An parameter contribution from each species.

Then the contribution to R1(Po),R2(Po) from the final atomic state: repeating the above procedure.

The values of the parameters R1(Po),R2(Po) for the initial and final states are summed.

Subroutine AS calculates the value of A^{j}_{*} as shown in the integrals on page 12 by performing a Hermite integration.
(* - defines what species is involved.)

Subroutine SUMRI is called separately to evaluate the imaginary and real parts of the function B at Hermite abscissa points.

Subroutine Herm is called to perform the integration.

Subroutine SUMRI calculates the real or imaginary part of the function B by evaluating the integrals as shown in equation III.8 . It performs a trapaziodal method of integration:

First it breaks the range of integration into one hundred steps.

At each point subroutine NBEQ is called to evaluate the function that is being integrated and the integral to that point is summed.

Subroutine NBEQ evaluates the function that is being integrated in equation III.8 at a specified integration point.

First it determines if its the real or imaginary part of the calculation since different formulas are required and then procedes to the apropriate part of the subroutine.

Subroutine KS is called to evaluate the appropriate value of $|K(Q)|^2$ as shown in equations III.11, III.12.

The appropriate value of $|K(Q)|^2$ is used to calculate B .

Subroutine KS calculates the value of $|K(Q)|^2$:

It determines what formulation for $|K(Q)|^2$ should be used.

For a charged particle equation III.11 is solved.

For a neutral particle equation III.12 is solved.

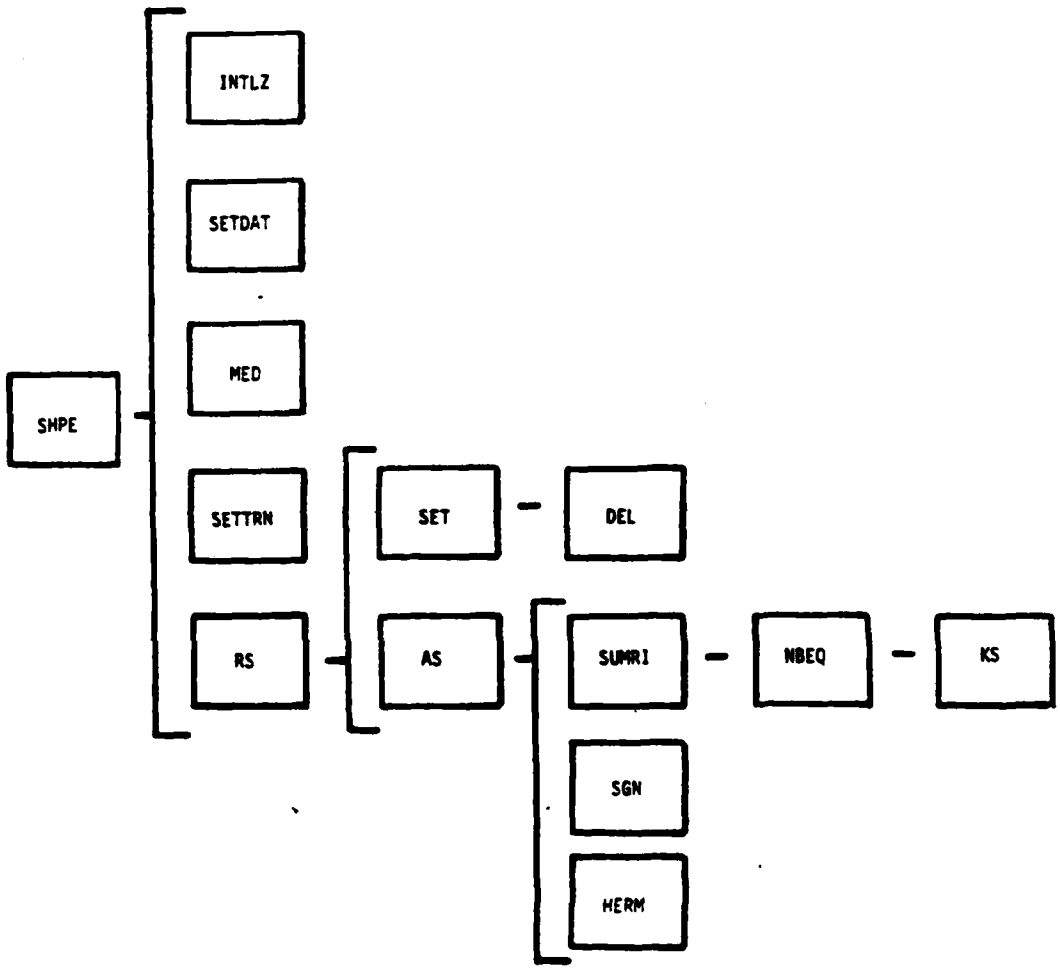


Figure 1. Flowchart for Subroutine SHPE

A.2 Computer Program Listing

```
      SUBROUTINE SHPE(ZRNGE,SHAPE,RHA,RHB,RHG,RHD,
     1                TEMA,TEMB,TEMG,TEMD,F0,IS,NZ)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /RSVAL/ R1(20),R2(20)
      COMMON /HERDAT/ HWT(20),HABS(20),NHERM
      COMMON /TRANS/ INIT,INITX,LAST,LASTX,DJE,DJN,
     1               GIN,GAME,SHIFTZ,NTRANS(50),NEXCIT(5),FRAC,IDK
      COMMON /CSNE/ AMASS,EMASS,GMASS,ZETA,RLJ
      COMMON /MEDM/ RHOA,RHOB,RHOG,RHOD,
     1              TA,TB,TG,TD,
     2              PA,PB,PG,PD,
     3              RKA,RKB,RKG,RKD
      COMMON /CONST/ E2,PI,VELC,RVKB,CONST1
      DIMENSION ZRNGE(NZ),SHAPE(NZ)
      DIMENSION F1(100)
C
C      SUBROUTINE SHPE -  DRIVING ROUTINE TO CALCULATE LINESHAPE
C
C     CALL INPUTS
C
C          ZRNGE(NZ) - ARRAY OF FREQUENCIES (     )
C          RH* - SPECIES DENSITY ( /CM3)
C          TEM* - SPECIES TEMPERATURE (DEG K)
C          (* = A(ATOM), B(ELECTRON), G(BUFFER), D(ION) )
C          F0 - BOHR FREQUENCY ( /CM)
C          IS - INDEX TO IDENTIFY TRANSITION
C          NZ - NUMBER OF FREQUENCIES
C
C     CALL OUTPUTS
C
C          SHAPE(NZ) - LINESHAPE
C
C      VARIABLES
C
C          ZETA - DOPPLER WIDTH ( /CM)
C          NTRANS(IS) - NUMBER OF  FINE STRUCTURE LINES
C
      DATA KALL/0/
      IF( KALL  .EQ.  1 ) GO TO 20
      KALL=1
      CALL INTLZ
      CALL SETDAT
   20 CONTINUE
      RHOA=RHA
```

```
      RHOB=RHB
      RHOG=RHG
      RHOD=RHD
      TA=TEMA
      TB=TEMB
      TG=TEMG
      TD=TEMD
      CALL MED
      ZETA=PA*2.0*PI*FO/(VELC*AMASS)
      NTRAN=NTRANS(IS)
      DO 50 IZ=1,NZ
      SHAPE(IZ)=0.0
   50 CONTINUE
C
C     LOOP OVER LINE TRANSITIONS
C
      DO 100 NT=1,NTRAN
      CALL SETTRN(NT,IS)
      CALL RS
      PRINT 1010,(R1(II),R2(II),II=11,20)
 1010 FORMAT(1X,1P10E12.2)
C
C     LOOP OVER FREQUENCY VALUES
C
      DO 200 IZ=1,NZ
      Z=ZRNGE(IZ)-SHIFTZ
      F1(IZ)=0.0
C
C     HERMITE INTEGRATION
C
      DO 300 IH=1,NHERM
      W=HABS(IH)
      WT=HWT(IH)
      IF(W.LT.0.0) GO TO 300
      F1(IZ)=F1(IZ)+W*(DATAN((Z+R1(IH)+ZETA*W)/R2(IH))
     1          -DATAN((Z+R1(IH)-ZETA*W)/R2(IH)))*WT
  300 CONTINUE
      SHAPE(IZ)=SHAPE(IZ)+F1(IZ)*FRAC
  200 CONTINUE
  100 CONTINUE
      RETURN
      END
      SUBROUTINE INTLZ
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /CSNE/ AMASS,EMASS,GMASS,ZETA,RLJ
```

```
      COMMON /CONST/ E2,PI,VELC,RVKB,CONST1
      COMMON /MEDM/ RHOA,RHOB,RHOG,RHOD,
     1              TA,TB,TG,TD,
     2              PA,PB,PG,PD,
     3              RKA,RKB,RKG,RKD
      COMMON /TRANS/ INIT,INITX,LAST,LASTX,DJE,DJN,
     1               GIN,GAME,SHIFTZ,NTRANS(50),NEXCIT(5),FRAC,IDK
C
C     *** EMASS - ELECTRON MASS (CM-1)
C     *** AMASS - ATOMIC MASS (CM-1)
C     *** GMASS - BUFFER MASS (CM-1)
C     *** CONSTI-
C     *** VELC  - VELOCITY LIGHT (CM/S)
C     *** RVKB  - BOLTZMANN CONSTANT
C
      E2=1.0/137.0
      EMASS=1.0/3.8616D-11
      AMASS=133.0*1836.0*EMASS
      GMASS=20.*1836.0*EMASS
      CONST1=6.73E-14
      VELC=3.0E10
      RVKB=1.3807D-16/1.9865D-16
      PI=3.14159265D0
      RETURN
      END
      SUBROUTINE SETDAT
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /TRANS/ INIT,INITX,LAST,LASTX,DJE,DJN,
     1               GIN,GAME,SHIFTZ,NTRANS(50),NEXCIT(5),FRAC,IDK
      COMMON /ATDAT/ NSHELL(60),LMO(60),JMO(60),EN(60),GAMARR(60)
      COMMON /CONST/ E2,PI,VELC,RVKB,CONST1
C
C      SUBROUTINE SETDAT - SETS ATOMIC DATA
C
C           NSHELL(I) - PRINCIPAL QUANTUM NUMBER
C           LMO(I)    - ORBITAL ANGULAR MOMENTUM
C           JMO(I)    - TOTAL ANGULAR MOMENTUM * 2
C           EN(I)     - ENERGY LEVEL OF STATE ( /CM)
C           GAMARR(I) - LIFETIME OF STATE ( /S)
C
      DATA NSHELL     /   6,   6,   6,   5,   5,   7,   7,   7,
     1                    6,   6,   8,   4,   4,   8,   8,   7,
     1                    7,   9,   5,   5,   5,   9,   9,   8,
     1                    8,  10,   6,   6,   6,   6,  10,  10,
     1                    9,   9,  11,   7,   7,  11,  11,  10,
```

```
     1                  10,   12,    8,    8,   12,   12,   11,   11,
     1                   9,    9,10*0/
      DATA LMO        /  0,    1,    1,    2,    2,    0,    1,    1,
     1                   2,    2,    0,    3,    3,    1,    1,    2,
     1                   2,    0,    3,    3,    4,    1,    1,    2,
     1                   2,    0,    3,    3,    4,    5,    1,    1,
     1                   2,    2,    0,    3,    3,    1,    1,    2,
     1                   2,    0,    3,    3,    1,    1,    2,    2,
     1                   3,    3,10*0/
      DATA JMO        /  1,    1,    3,    3,    5,    1,    1,    3,
     1                   3,    5,    1,    7,    5,    1,    3,    3,
     1                   5,    1,    7,    5,   79,    1,    3,    3,
     1                   5,    1,    7,    5,   79,  911,    1,    3,
     1                   3,    5,    1,    7,    5,    1,    3,    3,
     1                   5,    1,    7,    5,    1,    3,    3,    5,
     1                   7,    5,10*0/
      DATA EN         /      0.00D0,11178.24D0,11732.35D0,14499.49D0,
     1                  14597.08D0,18535.51D0,21765.65D0,21946.66D0,
     1                  22588.89D0,22631.83D0,24317.17D0,24472.29D0,
     1                  24472.46D0,25709.14D0,25791.78D0,26047.86D0,
     1                  26068.83D0,26910.68D0,26971.42D0,26971.56D0,
     1                  27010.00D0,27637.29D0,27681.96D0,27811.25D0,
     1                  27822.94D0,28300.28D0,28329.66D0,28329.76D0,
     1                  28347.00D0,28356.00D0,28727.09D0,28753.93D0,
     1                  28828.90D0,28836.06D0,29130.00D0,29148.16D0,
     1                  29148.23D0,29403.68D0,29421.10D0,29468.54D0,
     1                  29473.22D0,29666.00D0,29678.94D0,29678.98D0,
     1                  29852.85D0,29864.72D0,29896.64D0,29899.89D0,
     1                  30042.52D0,30042.54D0,10*0.D0/
      DATA GAMARR     / 0.       , 3.280D+07, 3.740D+07, 8.620D+05,
     1                  8.620D+05, 1.897D+07, 7.325D+06, 7.325D+06,
     1                  1.700D+07, 1.700D+07, 1.044D+07, 1.630D+07,
     1                  1.630D+07, 2.601D+06, 2.601D+06, 1.092D+07,
     1                  1.092D+07, 4.640D+06, 4.317D+06, 4.317D+06,
     1                  2.630D+06, 2.250D+05, 2.250D+05, 6.550D+05,
     1                  6.550D+06, 2.457D+06, 1.665D+06, 1.665D+06,
     1                  4.870D+05, 4.870D+05, 3.731D+06, 3.731D+06,
     1                  3.731D+06, 3.731D+06, 3.731D+06, 7.434D+05,
     1                  7.434D+05, 7.434D+05, 7.434D+05, 2.440D+06,
     1                  2.440D+06, 2.440D+06, 3.738D+05, 3.738D+05,
     1                  3.738D+05, 3.738D+05, 8.130D+05, 8.130D+05,
     1                  1.780D+05, 1.780D+05,10*0./
C
C      DIVIDE BY VELOCITY OF LIGHT - GAMARR(I) ( /CM)
C
```

```
      DO 200 N=1,60
      GAMARR(N)=GAMARR(N)/VELC
  200 CONTINUE
      RETURN
      END
      SUBROUTINE MED
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /CSNE/ AMASS,EMASS,GMASS,ZETA,RLJ
      COMMON /ATDAT/ NSHELL(60),LMO(60),JMO(60),EN(60),GAMARR(60)
      COMMON /TRANS/ INIT,INITX,LAST,LASTX,DJE,DJN,
     1               GIN,GAME,SHIFTZ,NTRANS(50),NEXCIT(5),FRAC,IDK
      COMMON /MEDM/ RHOA,RHOB,RHOG,RHOD,
     1              TA,TB,TG,TD,
     2              PA,PB,PG,PD,
     3              RKA,RKB,RKG,RKD
      COMMON /BCON/ RITAA,RITAB,RITAG,RITAD,
     1              EPSA,EPSB,EPSG,EPSD,
     2              RKSIA,RKSIB,RKSIG,RKSID,
     3              CJA,CJB,CJG,CJD,
     4              GAMJ,G,GP,DNPJ,DJ,LJ
      COMMON /CONST/ E2,PI,VELC,RVKB,CONST1
C
C     SUBROUTINE MED CALCULATES PARAMETERS WHICH REMAIN CONSTANT
C          THROUGH EACH CALL TO SUBROUTINE SHPE
C
C          P* - SPECIES MOMENTUM ( /CM)
C          RK* - RATIO OF MOMENTUM * RATIO OF MASS
C
C          (* = A(ATOM), B(ELECTRON), G(BUFFER), D(ION))
C
      PA=DSQRT(2.0*AMASS*RVKB*TA)
      PB=DSQRT(2.0*EMASS*RVKB*TB)
      PG=DSQRT(2.0*GMASS*RVKB*TG)
      PD=DSQRT(2.0*AMASS*RVKB*TD)
      RKA=1.0
      RKB=(PA/PB)*(EMASS/AMASS)
      RKG=(PA/PG)*(GMASS/AMASS)
      RKD=(PA/PD)*(AMASS/AMASS)
      RETURN
      END
      SUBROUTINE SETTRN(NT,IS)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /TRANS/ INIT,INITX,LAST,LASTX,DJE,DJN,
     1               GIN,GAME,SHIFTZ,NTRANS(50),NEXCIT(5),FRAC,IDK
      COMMON /ATDAT/ NSHELL(60),LMO(60),JMO(60),EN(60),GAMARR(60)
```

```
ION I1(3,50),I2(3,50),I3(3,50),I4(3,50),I5(5,50)
ION R1(3,50),R2(3,50),R3(3,50)
ION NXTRAN(50)

TINE SETTRN - SET TRANSITION INDICES

INPUTS

S - INDEX TO IDENTIFY TRANSITION
T - NUMBER OF THE FINE STRUCTURE TRANSITION INVOLVED

BLES

NTRANS(IS) - NUMBER OF TRANSITIONS WITHOUT EXCITATION
NXTRAN(IS) - NUMBER OF TRANSITIONS DUE TO EXCITATION
I1(I,IS)   - INDEX IDENTIFYING INITIAL STATE
I2(I,IS)   - INDEX OF PERTURBING FINE STRUCTURE LINE
I3(I,IS)   - INDEX OF FINAL STATE
I4(I,IS)   - INDEX OF PERTURBING FINE STRUCTURE LINE
I5(I,IS)   - INDEX OF EXCITING STATE
R1(I,IS)   - DIPOLE MATRIX ELEMENT SQUARED- INITIAL
R2(I,IS)   - DIPOLE MATRIX ELEMENT SQUARED- FINAL
R3(I,IS)   - DIPOLE MATRIX ELEMENT SQUARED- GROUND

TRANS(18)/3/
XTRAN(18)/1/
1(1,18),I1(2,18),I1(3,18)/19,20,20/
2(1,18),I2(2,18),I2(3,18)/20,19,19/
3(1,18),I3(2,18),I3(3,18)/05,05,04/
4(1,18),I4(2,18),I4(3,18)/04,04,05/
5(1,18),I5(2,18)/21,0/
1(1,18),R1(2,18),R1(3,18)/3*3.15E-14/
2(1,18),R2(2,18),R2(3,18)/3*1.14E-15/
3(1,18),R3(2,18),R3(3,18)/3*6.4E-16/
TRANS(24)/3/
XTRAN(24)/0/
1(1,24),I1(2,24),I1(3,24)/13,13,12/
2(1,24),I2(2,24),I2(3,24)/12,12,13/
3(1,24),I3(2,24),I3(3,24)/05,04,05/
4(1,24),I4(2,24),I4(3,24)/04,05,05/
1(1,24),R2(2,24),R3(2,24)/3*2.0D-14/
2(1,24),R2(2,24),R2(3,24)/3*1.14D-15/
3(1,24),R3(2,24),R3(3,24)/3*6.4D-16/
I(NT,IS)
I2(NT,IS)
```

```
      NXT=NXTRAN(IS)
      DO 10 IX=1,NXT
      NEXCIT(IX)=I5(IX,IS)
   10 CONTINUE
      LAST=I3(NT,IS)
      LASTX=I4(NT,IS)
      DJE=R1(NT,IS)
      DJN=R2(NT,IS)
      GIN=R3(NT,IS)
      GAME=GAMARR(INIT)
      ZCINIT=(EN(I1(1,IS))+EN(I2(1,IS)))/2.0
      ZCLAST=(EN(I3(1,IS))+EN(I4(1,IS)))/2.0
      SHIFTZ=EN(INIT)-ZCINIT+ZCLAST-EN(LAST)
      DENOM=2.0*(2.0*(DFLOAT(LMO(INIT))+1.0))
      FRAC=(DFLOAT(JMO(INIT))+1.0)/DENOM
      IDK=0
      IF(LMO(INIT).NE.LMO(INITX))IDK=1
      RETURN
      END
      SUBROUTINE RS
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /TRANS/ INIT,INITX,LAST,LASTX,DJE,DJN,
     1               GIN,GAME,SHIFTZ,NTRANS(50),NEXCIT(5),FRAC,IDK
      COMMON /HERDAT/ HWT(20),HABS(20),NHERM
      COMMON /CSNE/ AMASS,EMASS,GMASS,ZETA,BLJ
      COMMON /RSVAL/ R1(20),R2(20)
      COMMON /MEDM/ RHOA,RHOB,RHOG,RHOD,
     1              TA,TB,TG,TD,
     2              PA,PB,PG,PD,
     3              RKA,RKB,RKG,RKD
      COMMON /BCON/ RITAA,RITAB,RITAG,RITAD,
     1              EPSA,EPSB,EPSG,EPSD,
     2              RKSIA,RKSIB,RKSIG,RKSID,
     3              CJA,CJB,CJG,CJD,
     4              GAMJ,G,GP,DNPJ,DJ,LJ
      DIMENSION R1E(20),R2E(20),R1N(20),R2N(20)
C
C     SUBROITINE RS - CALCULATES LINESHAPE PARAMETERS R1,R2
C
C     VARIABLES
C
C         R1E(IH),R2E(IH) - LINESHPAE PARAMETER INITIAL STATE
C         R1N(IH),R2N(IH) - LINESHAPE PARAMETER FINAL STATE
C         IEXCIT          - INDEX FOR EXCITED STATES
C         GAME            - RADIATIVE WIDTH
```

```
C
      IEXCIT=0
      DO 50 IH=1,NHERM
      R1(IH)=0.0
      R2(IH)=0.0
      R1E(IH)=0.0
      R2E(IH)=0.0
      R1N(IH)=0.0
      R2N(IH)=0.0
   50 CONTINUE
   60 IEXCIT=IEXCIT+1
      IF(IEXCIT.GT.1)INITX=NEXCIT(IEXCIT-1)
      IF( INITX  .EQ.  0 ) GO TO 150
C
C     *** INITIAL STATE
C
      CALL SET(INIT,INITX,DJE,GIN)
      DO 100 IH=1,NHERM
      W=HABS(IH)
      IF(W.LT.0.0) GO TO 100
      CALL AS(W,RITAA,EPSA,RKSIA,RKA,CJA,1,ARA,AIA)
      CALL AS(W,RITAB,EPSB,RKSIB,RKB,CJB,2,ARB,AIB)
      CALL AS(W,RITAG,EPSG,RKSIG,RKG,CJG,3,ARG,AIG)
      CALL AS(W,RITAD,EPSD,RKSID,RKD,CJD,4,ARD,AID)
      R1E(IH)=R1E(IH)+ARA+ARB+ARG+ARD
      R2E(IH)=R2E(IH)+AIA+AIB+AID+AID
      PRINT 1010,R1E(IH),ARA,ARB,ARG,ARD,R2E(IH),AIA,AIB,AIG,AID
 1010 FORMAT (1X,1H+,1P10E12.2)
  100 CONTINUE
      GO TO 60
  150 CONTINUE
C
C     *** FINAL STATE
C
      CALL SET(LAST,LASTX,DJN,GIN)
      DO 200 IH=1,NHERM
      W=HABS(IH)
      IF( W  .LT.  0.0 ) GO TO 200
      CALL AS(W,RITAA,EPSA,RKSIA,RKA,CJA,1,ARA,AIA)
      CALL AS(W,RITAB,EPSB,RKSIB,RKB,CJB,2,ARB,AIB)
      CALL AS(W,RITAG,EPSG,RKSIG,RKG,CJG,3,ARG,AIG)
      CALL AS(W,RITAD,EPSD,RKSID,RKD,CJD,4,ARD,AID)
      R1N(IH)=ARA+ARB+ARG+ARD
      R2N(IH)=AIA+AIB+AID+AID
      PRINT 1020,R1N(IH),ARA,ARB,ARG,ARD,R2N(IH),AIA,AIB,AIG,AID
```

```
 1020 FORMAT(1X,1H-,1P10E12.2)
  200 CONTINUE
      DO 300 IH=1,NHERM
      W=HABS(IH)
      IF(W.LT.0.0) GO TO 300
      R1(IH)=R1E(IH)-R1N(IH)
      R2(IH)=GAME/2.0+R2E(IH)+R2N(IH)
  300 CONTINUE
      RETURN
      END
      SUBROUTINE SET(IDJ,IDJX,DJT,GIN)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /ATDAT/ NSHELL(60),LMO(60),JMO(60),EN(60),GAMARR(60)
      COMMON /MEDM/ RHOA,RHOB,RHOG,RHOD,
     1              TA,TB,TG,TD,
     2              PA,PB,PG,PD,
     3              RKA,RKB,RKG,RKD
      COMMON /BCON/ RITAA,RITAB,RITAG,RITAD,
     1              EPSA,EPSB,EPSG,EPSD,
     2              RKSIA,RKSIB,RKSIG,RKSID,
     3              CJA,CJB,CJG,CJD,
     4              GAMJ,G,GP,DNPJ,DJ,LJ
      COMMON /CSNE/ AMASS,EMASS,GMASS,ZETA,RLJ
      COMMON /CONST/ E2,PI,VELC,RVKB,CONST1
C
C     SUBROUTINE SET - SETS CONSTANTS THAT DEPEND ON WHICH TRANSITION IS
C           TRANSITION IS BEING EVALUATED
C
C          CALL INPUTS
C
C               IDJ  - INDEX OF PRIMARY STATE
C               IDJX - INDEX OF PERTURBING STATE
C               DJJ  - DIPOLE MATRIX ELEMENT SQUARED
C               GIN  - DIPOLE MATRIX ELEMENT SQUARED - GROUND
C
C          VARIABLES
C
C               RITA*  - OFF RESONANT ENERGY PARAMETER
C               EPS*   - DECAY WIDTH PARAMETER
C               RKSI*  - MATRIX ELEMENT PARAMETER
C               CJ*    - COUPLING STRENGTH
C
      FACTP=(2.0*PI)**2.5
      GAMJ=GAMARR(IDJ)
      G=GIN
```

```
      GP=G/30.
      DJ=DJT
      DNPJ=DEL(IDJX,IDJ)
      LJ=LMO(IDJ)
      RLJ=DFLOAT(LJ)
C
C     *** ATOM-ATOM
C
      RITAA=AMASS*DNPJ*DJ/12.
      EPSA=-AMASS*GAMJ*DJ/24.
      RKSIA=PA*DSQRT(DJ/12.)
      CJA=108.*E2*E2*AMASS*G*G*RHOA/(FACTP*DJ*PA)
C
C     *** ELECTRON - ATOM
C
      RITAB=EMASS*DNPJ*DJ/6.
      EPSB=-EMASS*GAMJ*DJ/12.
      RKSIB=PB*DSQRT(DJ/12.)
      CJB=3.*E2*E2*AMASS*DJ*RHOB/(FACTP*PA)
C
C     *** BUFFER - ATOM
C
      RITAG=GMASS*DNPJ*DJ/6.
      EPSG=-GMASS*GAMJ*DJ/12.
      RKSIG=PG*DSQRT(DJ/12.)
      CJG=108.*E2*E2*AMASS*GP*GP*RHOG/(FACTP*PA*DJ)
C
C     *** ION - ATOM
C
      RITAD=AMASS*DNPJ*DJ/12.
      EPSD=-AMASS*GAMJ*DJ/24.
      RKSID=PD*DSQRT(DJ/12.)
      CJD=3.*E2*E2*AMASS*DJ*RHOD/(FACTP*PA)
      RETURN
      END
      FUNCTION DEL(N1,N2)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /ATDAT/ NSHELL(60),LMO(60),JMO(60),EN(60),GAMARR(60)
      COMMON /CONST/ E2,PI,VELC,RVKB,CONST1
C
C     DEL(N1,N2) = BOHR FREQUENCY ( /CM)
C
C      N1,N2 - INDICIES OF ATOMIC ENERGY LEVELS
C
      DEL=(EN(N1)-EN(N2))*(2.0*PI)
```

```
      RETURN
      END
      SUBROUTINE AS(W,RITA,EPS,RKSI,RK,CJ,ID,AR,AI)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /HERDAT/ HWT(20),HABS(20),NHERM
      DIMENSION F1(20),F2(20)
C
C     SUBROUTINE AS - CALCULATES DENSITY INDEPENDENT
C                     LINESHAPE PARAMETER
C
C          CALL INPUTS
C
C              W    - HERMITE ABSCISSA VALUE
C              RITA - OFF RESONANT ENERGY PARAMETER
C              EPS  - DECAY WIDTH PARAMETER
C              RKSI - MATRIX ELEMENT PARAMETER
C              RK   - RATIO OF MOMENTUM & RATIO MASS
C              CJ   - COUPLING STRENGTH
C              ID   - INDEX TO IDENTIFY SPECIES
C
C          CALL OUTPUTS
C
C              AR   - REAL PART DENS INDEP LINESHAPE PARAM
C              AI   - IMAG PART DENS INDEP LINESHAPE PARAM
C
      DO 100 IH=1,NHERM
      V=HABS(IH)
      VW=V+RK*W
      X=DABS(VW)
      CALL SUMRI(0.D0,X,X,RITA,EPS,RKSI,ID,0,VALI)
      CALL SUMRI(-1.D0,1.D0,X,RITA,EPS,RKSI,ID,1,VALR)
      F1(IH)=SGN(VW)*VALR
      F2(IH)=SGN(VW)*VALI
  100 CONTINUE
      CALL HERM(F1,AR)
      CALL HERM(F2,AI)
      AR=CJ*AR/W
      AI=CJ*AI/W
      RETURN
      END
      SUBROUTINE SUMRI(YL,YU,X,RITA,EPS,RKSI,ID,IR,VAL)
      IMPLICIT REAL*8(A-H,O-Z)
C
C     SUBROUTINE SUMRI - PERFORMS A TRAPAZOIDAL INTEGRATION
C                      - THE FUNCTION INTEGRATED IS EVALUATED
```

```
C                        IN SUBROUTINE NBEQ
C
C          CALL INPUTS
C
C               YL    - LOWER LIMIT INTEGRATION
C               YU    - UPPER LIMIT INTEGRATION
C               X     - ABSCISSA VALUE
C               RITA  - OFF RESONANT ENERGY PARAMETER
C               EPS   - DECAY WIDTH PARAMETER
C               RKSI  - MATRIX ELEMENT PARAMETER
C               ID    -  IDENTIFY SPECIES
C               IR    - IDENTIFY REAL OF IMAGINARY
C
C          CALL OUTPUTS
C
C               VAL   -  VALUE OF INTEGATION
C
      DATA NINT/100/
      DY=(YU-YL)/DFLOAT(NINT)
      VAL=0.0
      Y=YL
      CALL NBEQ(X,Y,RITA,EPS,RKSI,ID,IR,BVAL)
      NB=NINT
      BL=BVAL
      DO 100 IN=1,NINT
      Y=Y+DY
      CALL NBEQ(X,Y,RITA,EPS,RKSI,ID,IR,BVAL)
      VAL=VAL+(BVAL+BL)/2.0
      BL=BVAL
  100 CONTINUE
      VAL=VAL*DY
      RETURN
      END
      SUBROUTINE NBEQ(X,Y,RITA,EPS,RKSI,ID,IR,BVAL)
      IMPLICIT REAL*8(A-H,O-Z)
C
C     SUBROUTINE NBEQ - EVALUATES B FUNCTION
C                     - THE INTERACTION PARAMETER
C
C           CALL INPUTS
C
C                X    - ABSCISSA VALUE
C                Y    - CURRENT INTEGRATION ABSCISSA
C                RITA - OFF RESONANT ENERGY PARAMETER
C                EPS  - DECAY WIDTH PARAMETER
```

```
C                RKSI - MATRIX ELEMENT PARAMETER
C                ID   - INDEXIDENTIFIES SPECIES
C                IR   - INDEX IDENTIEFIES REAL OR IMAGINARY PART
C
C           CALL OUTPUTS
C
C                BVAL - VALUE OF INTERACTION PARAMETER
C
      BVAL=0.
      IF(IR.EQ.1)GO TO 100
      FAC=Y*Y-RITA/(RKSI*RKSI)
      IF(FAC.LT.0.)RETURN
      RT=DSQRT((RKSI*Y)**2-RITA)
      QP=-RKSI*Y+RT
      QM=-RKSI*Y-RT
      CALL KS(QP,QPK,ID)
      CALL KS(QM,QMK,ID)
      BVAL=1.0/DSQRT(FAC)*(QP*QP*QPK+QM*QM*QMK)
      RETURN
  100 CONTINUE
      CALL KS(Y,YK,ID)
      BVAL=Y*YK*DLOG((Y*Y+2.0*RKSI*X*Y+RITA*RITA)**2+EPS*EPS)
      RETURN
      END
      SUBROUTINE KS(Y,VALK,ID)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /CSNE/ AMASS,EMASS,GMASS,ZETA,RLJ
      COMMON /TRANS/ INIT,INITX,LAST,LASTX,DJE,DJN,
     1               GIN,GAME,SHIFTZ,NTRANS(50),NEXCIT(5),FRAC,IDK
      COMMON /BCON/ RITAA,RITAB,RITAG,RITAD,
     1              EPSA,EPSB,EPSG,EPSD,
     2              RKSIA,RKSIB,RKSIG,RKSID,
     3              CJA,CJE,CJG,CJD,
     4              G4MJ,G,GF,DNFJ,DJ,LJ
C
C     SUBROUTINE KS - EVALUATES INTERACTION KERNAL
C
C           CALL INPUTS
C
C                Y  - ABSCISSA VALUE
C                ID - INDEX TO IDENTIFY SPECIES
C
C           CALL OUTPUTS
C
C                VALK - VALUE OF INTERACTION KERNAL
```

```
C
      DATA FAIL/1.E-3/
      FAC=0.
      IF(Y.NE.0.)FAC=1./(Y*Y)
      IF(DABS(Y).LE.FAIL)FAC=0.0
      IF(ID.EQ.1)GO TO 100
      IF(ID.EQ.3)GO TO 100
C
C     *** CHARGED SPECIES INTERACTION
C
      B=GAMJ*DSQRT(DJ/6.)
      POWER=(-2.0*(RLJ+3.0)*DLOG(1.0+Y*Y))
      VALK=DEXP(POWER)
      IF(IDK.EQ.1)VALK=FAC*VALK
      RETURN
  100 CONTINUE
C
C     *** NEUTRAL SPECIES INTERACTION
C
      IF(ID.EQ.1)H=G/DJ
      IF(ID.EQ.3)H=G/(30.*DJ)
      POWER=(-2.0*(RLJ+3.0)*DLOG(1.0+Y*Y)-6.0*
     $DLOG(1.0+H*Y*Y))
      VALK=Y**4*DEXP(POWER)
      IF(IDK.EQ.1)VALK=VALK*FAC
      RETURN
      END
      FUNCTION SGN(A)
      IMPLICIT REAL*8(A-H,O-Z)
      SGN=0.0
      IF( A  .EQ.  0 ) RETURN
      SGN=A/DABS(A)
      RETURN
      END
      SUBROUTINE HERM(F,VAL)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /HERDAT/ HWT(20),HABS(20),NHERM
      DIMENSION F(20)
C
C     *** HERMITE INTEGRATION
C
C     *** F - FUNCTION TO BE INTEGRATED
C     ***     EVALUATED AT ABSCISSA VALUES HABS(IX)
C     *** VAL - INTEGRATED VALUE
C
```

```
      DATA HWT/2.2293936455D-13,4.3993409922D-10,1.0860693707D-07,
     $         7.8025564785D-06,2.2833863601D-04,3.2437733422D-03,
     $         2.4810520887D-02,1.0901720602D-01,2.8667550536D-01,
     $         4.6224366960D-01,4.6224366960D-01,
     $         2.8667550536D-01,1.0901720602D-01,2.4810520887D-02,
     $         3.2437733422D-03,2.2833863601D-04,7.8025564785D-06,
     $         1.0860693707D-07,4.3993409922D-10,2.2293936455D-13/
      DATA HABS/-5.3874808900D0,-4.6036824495D0,-3.9447640401D0,
     $          -3.3478545673D0,-2.7888060584D0,-2.2549740020D0,
     $          -1.7385377121D0,-1.2340762153D0,-0.7374737285D0,
     $          -0.2453407083D0,+0.2453407083D0,
     $          +0.7374737285D0,+1.2340762153D0,+1.7385377121D0,
     $          +2.2549740020D0,+2.7888060584D0,+3.3478545673D0,
     $          +3.9447640401D0,+4.6036824495D0,+5.3874808900D0/
      DATA NHERM /20/
      DATA NHER2 /10/
      VAL=0.0
      DO 100 IX=1,NHER2
      VAL=VAL+HWT(IX)*(F(IX)+F(NHERM+1-IX))
  100 CONTINUE
      RETURN
      END
```

END

FILMED

8-83

DTIC